

# Induced polarization and electronic properties of carbon doped boron-nitride nanoribbons

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The electronic properties of boron-nitride nanoribbons (BNNRs) doped with a line of carbon atoms are investigated by using density functional calculations. Three different configurations are possible: the carbon atoms may replace a line of boron or nitrogen atoms or a line of alternating B and N atoms which results in very different electronic properties. We found that: i) the NCB arrangement is strongly polarized with a large dipole moment having an unexpected direction, ii) the BCB and NCN arrangement are non-polar with zero dipole moment, iii) the doping by a carbon line reduces the band gap independent of the local arrangement of boron and nitrogen around the carbon line, iv) an electric field parallel to the carbon line polarizes the BN sheet and is found to be sensitive to the presence of carbon dopants, and v) the energy gap between the highest occupied molecular orbital and the lowest unoccupied molecular orbital decreases linearly with increasing applied electric field directed parallel to the carbon line. We show that the polarization and energy gap of carbon doped BNNRs can be tuned by an electric field applied parallel along the carbon line.

Single layer hexagonal boron-nitride (h-BN) nanosheets have been recently produced and placed on top of a SiO<sub>2</sub> substrate [1]. Several experimental groups have also fabricated free-standing h-BN single layers using sputtering of controlled energetic electron beams [2, 3]. Unlike graphene, a h-BN sheet is a wide gap insulator, as is hexagonal BN, which is a promising material for opto-electronic technologies [4, 5], tunnel devices and field-effect transistors [6, 7]. Small flakes of h-BN, i.e. BN nanoribbons (BNNRs), are semiconductors when hydrogen-passivated on one of the edges [8–10]. The band gap of BNNR can be tuned by using different types of atoms for edge passivation [11–14]. The zigzag BNNR has half-metallic properties when the boron edge is hydrogen-passivated, and the nitride edge is bare [11]. Under a hydrogen-rich environment, the zigzag BNNR with two-hydrogen-terminated edges becomes a ferromagnetic metal [14]. Moreover, the electronic and magnetic properties of the BNNRs could be modulated by applying an extra transversal electric field. Zhang *et al* used the local density approximation (LDA) to study the energy gap and showed that it can be tuned by applying a transverse electric field on a semi-infinite hydrogen passivated BNNRs with zigzag or armchair edges [9]. Similarly by using the LDA, Park *et al* found that a transverse electric field decreases the band gap of armchair BNNRs monotonically while the band gap of zigzag BNNRs either increases or decreases depending on the direction and the strength of the applied field [10]. Additionally, random doping BN with C atoms leads to spontaneous magnetization [15, 16]. Sai *et al* found piezoelectricity in a heteropolar nanotube depending on the chirality and diameter of the nanotube

which originates from the piezoelectric response of an isolated planar BN sheet [17].

In this study, we report first-principles calculations for the BNNRs which are doped by a *zigzag line of carbon atoms* in the middle and passivated by hydrogen atoms at the edges. We study different possible positions of the line of carbon atoms with respect to the BN-lattice and found that piezoelectricity and consequently the permanent polarization in the BNNRs can be strongly enhanced, tuned or even eliminated depending on the type of atoms (B or N) that surrounds the dopants. We found that doping BNNRs by carbon atoms decreases the band gap while the electric polarization of the doped BNNRs depends on the type of atoms (B or N) that surrounds the dopants. The NCB system is polarized in an unexpected way while BCB and NCN have zero dipole moments. We find that an external planar electric field applied along the C-line either reduces or increases the band gap and the dipole moment depending on its direction.

## Model and Method

Our system is a finite-size h-BN sheet which is passivated by hydrogens at its edges. A rectangular h-BN ribbon  $3.1 \times 3.4 \text{ nm}^2$  in size is taken as a perfect nanoribbon, see Fig. 1. Total number of B and N atoms in the sheet is 418, in addition there are 56 H atoms at the edges. A zigzag line of 28 atoms is inserted in the middle of the system replacing a line of h-BN atoms. We have studied three different positions of the carbon line (C-line) with respect to the BN-lattice as illustrated in Figs. 1(b-d) and compare the results with the undoped sheet (Fig. 1(a)). Three different ways of inserting the central C-line are: i) a C-line in the center with boron and nitrogen atoms on both sides (Fig. 1(b)) which we name NCB, ii) a C-line in the center with boron atoms on both sides (Fig. 1(c)) which we name BCB, iii) a C-line in the center with nitrogen atoms on both sides (Fig. 1(d)) which we name NCN. Notice that all these systems are

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passivated by hydrogen atoms at the edges to saturate the edge chemical bonds. In order to have equal sizes on both sides of the C-line, one has to simulate a non-exact rectangular flake, i.e. the right-up and down-left corners are not orthogonal, as illustrated by the two dashed rectangles in Fig. 1(b) having the same size. Therefore in the RHS (LHS) rectangles in NCB, BCB and NCN there are additional B(N), B(B), N(N) atoms, respectively (see Figs. 1(c-d)).

We employ density functional theory as implemented in GAUSSIAN (G09) [18] which is an electronic structure packages that uses a basis set of Gaussian type of orbitals. For the exchange and correlation (XC) functional, the hybrid functional B3LYP is adopted in G09. For some particular cases, and for comparison purposes, we also used the LDA as implemented in the BigDFT [19] package which uses real-space wavelets. In both cases, the self consistency loop iterates until the change in the total energy is less than  $10^{-7}$  eV, and the geometries are considered relaxed once the force on each nucleus is less than 50 meV/Å. Using the 6-31G\* basis set in G09, we expect that our calculation is capable to provide a reliable description of the electronic properties of the different systems. Natural bonding orbital (NBO) analysis [20] is also performed at the B3LYP/6-31G\* level of theory [18].

### **Lattice mismatch**

We recall that in bulk h-BN the in-plane B-N bond length  $d_{BN} = 1.446\text{Å}$  has been determined by X-ray scattering [21]. Early ab-initio calculations [22] yielded  $d_{BN} = 1.35\text{Å}$ . We obtain  $d_{BN} = 1.45\text{Å}$  which agrees much better with experiment. On the other hand the bond lengths  $d_{NC}$  and  $d_{BC}$  between the inserted C-line atoms and the N and B surrounding atoms, as well as the intra-chain bond length  $d_{CC}$  between C-atoms, depend on the specific configuration of the atoms in the NCB, BCB and NCN systems (see Fig. 1). We summarized the results of our calculations in Table I. We found for the three doped BNNRs that  $d_{CC} < d_{BN} < d_{BC}$ . Notice that the relative sheet bond lengths  $d_{NC} = 1.41\text{Å}$  and  $1.43\text{Å}$  in NCB and NCN, respectively, are an indication of the partially double bond character of the N-C bonds at the central C-line is remarkable. The difference in bond lengths around the C-line in NCB are clearly visible in Fig. 1(b). The values  $d_{BC} = 1.55\text{Å}$  and  $d_{NC} = 1.41\text{Å}$  lead to a lattice mismatch and symmetry breaking between the left and the right part of our system along the inserted C-line. In Fig. 2, the arrows show the corresponding atomic displacement pattern for NCB. On the other hand the systems BCB and NCN (Figs. 1 (c,d)) are symmetric with respect to the C-line. The changes in the bond-length and the dependence of the configuration on the interface leads to changes in the electronic polarization and consequently to a piezoelectricity effect. The results of this electro-mechanical coupling will be discussed in the following part of this section.

### **Electronic charge distribution**

The perfect infinite BN sheet is a neutral sheet with

a uniform charge distribution far from the edges. Indeed, in an infinite two dimensional h-BN sheet the point group symmetry is  $D_{3h}$  and there is no permanent dipole moment. However in finite BNNRs structure the symmetry is broken which allows piezoelectricity, i.e. the appearance of a dipole under mechanical deformation. Therefore, the h-BN sheet is the most simple crystalline structure which allows piezoelectricity [23, 24]. On the other hand, in BNNRs the finite extension of the sheet and the passivation of the boundaries by H atoms lead to the appearance of a permanent dipole moment. For the case of BN (see Fig. 1(a)) using B3LYP we obtain a dipole moment  $\vec{P}_0 = (-10.58, -1.98)\text{D}$ , (in this study the electric dipole moment vectors point from the negative charge to the positive charge, e.g. see red arrow in Fig. 1(a)), i.e. the system becomes piezoelectric. In the following we investigate the influence of carbon doping on the polarization in BNNRs.

Inserting of C-line alters the charge distribution mostly in the neighborhood of the C-line (see Table I), while further away the charge distribution approaches the one of a perfect BNNR. The different values of electronegativity for B( $\approx 2.0$ ), C( $\approx 2.6$ ) and N( $\approx 3.0$ ) largely account for the charge redistribution and the concomitant formation of local dipoles.

For the NCB the local dipoles for B-C and C-N bonds around the carbon line are directed to the right (Fig. 1(b)) which polarized NCB. Surprisingly, although local dipoles are in the  $x$ -direction, we found that the total dipole moment is mainly in the  $y$ -direction (parallel to the carbon line), i.e. using B3LYP we find  $\vec{P}_0 = (-9.37, -42.89)\text{D}$ . We attribute this effect to the presence of carbon atoms in the middle of Fig. 1(b). The C atoms which are bonded to the B (N) atoms absorb (give) electronic charge yielding two different group of C atoms, i.e. those bonded to B atoms with negative electronic charge and those bonded to N atoms with positive electronic charge. This is the main reason for the unusual direction of the dipole moment. In fact the magnitude of  $P_y$  is related to the carbon line. Notice that this is seen only when different types of atoms surround the C-line, i.e. the BCB and NCN systems have small  $P_x$  and  $P_y$ .

As seen from Figs. 1(c,d) in the BCB and NCN systems the dipoles of the left and right hand sides of the C-line are in opposite directions and no overall dipole moment in the  $x$ -direction arises from these edges. There is a small dipole moment  $P_y$  because the corners are differently terminated at the left and right edges.

A similar description is possible for the strong local dipoles on the B-C and N-C bonds induced by the insertion of the C-line. Although having a C-line in the middle, the BCB and NCN systems have vanishing dipole moments in the  $x$ -direction because the local dipoles on the B-C and N-C bonds around the C-line are directed oppositely. The direction of the local dipole moments, indicated by the horizontal black arrows in Figs. 1(b-d), is chosen according to the electronegativity differences of the atoms as discussed earlier. It is important to note

that the number and arrangement of hydrogen atoms are the same in all model systems, thus the main reason of the strong total polarization is the local arrangement of B and N atoms around the C-line and not the presence of the H-atoms of the edges.

### ***Electrostatic potential***

The electrostatic potential (ESP) mapped on the plane of the h-BN sheet for the representative models is shown in Fig. 3. The sign of ESP at any point depends on whether the ESP due to the nuclei and the electrons is dominant at that point. The difference in electronegativity between the B and N atoms results in a combination of weak ionic and covalent bonding in the h-BN sheet. Fig. 3(a) shows that the B-N bonds have a larger ESP (blue spots) around the B ions as compared to the N sites (red spots). It shows that the N ions attract electronic charge from the B ions as one expects in view of the atomic electronegativities. A characteristic pattern of alternating positive and negative ESP regions is seen over the BN surface in which the left side has generally less ESP than the right side. Accordingly, this explains why the BN has a permanent dipole moment in accordance of the electronegativity differences on H-B and H-N bonds at the edge which saturate the dangling bonds. The NCB, as shown in Fig. 3(b), has a steep gradient in the ESP near the C-line which results in a strong dipole in this region which confirms the direction of the dipole moment shown in Fig. 1(b). The big arrows in Figs. 3(a,b) refer to the dipole moments. Similarly, the direction of the opposite dipoles in Figs. 1(c,d) can be well explained by the ESP variation in Figs. 3(c,d). Strong variation of the ESP around the carbon lines causes strong dipoles but directed oppositely. In NCB, the antisymmetrical distribution is also due to the chosen non-perfect geometry of the corners.

### ***Polarizability***

The polarization of the BNNR system varies in response to an external electric field. Here we focus on the NCB system which has an appreciable permanent polarization. We apply a uniform electric field in the plane of the flakes parallel to the C-line ( $y$ -direction) and allow them to relax each time the electric field is altered. The reason for directing the field along  $y$  is that we want to compensate the largest component of the spontaneous dipole moment  $P_0$ , i.e.  $P_y$ . The field strength  $E \equiv E_y$  is then increased step-wise until the induced dipole moment completely compensates  $P_y$ . We denote the compensating field strength by  $E_0$ . We also inverted  $E_y$  to check the linear dependence. Red symbols in Fig. 4 (for NCB system) show that the dipole moment has almost a linear dependence on  $E$  within the studied range (-1,0.8) V/nm. The slope of this line gives the polarizability  $\alpha_{yy} = dE/dP_y$ . From B3LYP we found  $\alpha_{yy}=45.66$  D nm/V and  $E_0 \approx 1$  V/nm. In Figs. 4(b,c) we show the ESP and  $P_0$  for  $E_y=-1.0$  V/nm and  $E_y=+0.82$  V/nm, respectively. The lattice deformations due to applied electric field are shown in Figs. 4(d,e). It is interesting to note that a positive electric field shifts the RHS-atoms

to the bottom and the LHS-atoms to the top, and vice versa for negative field. This yields a shear stress along the C-line (filled black symbols). The larger the electric field the larger deformation and the larger the enhancement of piezoelectricity.

### ***Metallic Properties***

To show the effect of the insertion of the C-line on the conductivity of BNNRs, we have listed the calculated energy gaps for our systems in Table I. The gap is calculated as the energy difference between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). It is well known that LDA (which we used in our BigDFT calculations) underestimates the energy of the excited levels and therefore the HOMO-LUMO gap. The hybrid functional B3LYP is expected to give a better estimation. However, both approximations reveal the same trend i.e. significant decrease in the HOMO-LUMO gap after insertion of the C-line. It implies that the electric conductivity is increased in the doped sheets, however their gaps are still large and therefore the system is not metallic. We will show later that the HOMO-LUMO gap can also be tuned by an electric field. Figure 5 illustrates the density of states (DOS) for the studied BNNRs according to B3LYP. Note that the insertion of a C-line generates a few new electronic states within the wide gap between the HOMO and LUMO of the perfect BN, reducing the gap width significantly. Notice that the distribution of energy levels around the HOMO-LUMO levels in BCB and NCN are different and the energy levels for NCN (BCB) are significantly separated below (above) the HOMO (LUMO).

The change in the metallic properties can be explained by looking at the distribution of the electronic states near the Fermi level. As seen from Fig. 3 in the BN system the HOMO (LUMO) is localized at two corners around the N (B) atoms. In the BN system, the HOMO is localized at the right-down side with zig-zag edges while the LUMO is localized at the left-upper corner with zig-zag edges where these corners are orthogonal opposite to the other corners, i.e. right-up and down-left with zig-zag edges. It shows that both chirality and the local geometry of the edges are important parameters for localizing the electrons. On the other hand in the doped systems the HOMO and LUMO states are localized around the C-line over either B-C or N-C bonds, see Figs. 3(b,c). In BCB and NCN systems the C-line opens a wide channel of few atoms through which the electronic charge can be transmitted. But the conductivity in the direction perpendicular to the C-line is expected to be small because no contribution from HOMO and LUMO is extended along this direction. Notice that the localized orbitals in BCB and NCN have different patterns. In BCB both HOMO and LUMO are localized on the C atoms and the adjacent B atoms (i.e. on the B-C bonds), while the N atoms are not contributing. This is apparently in contrast to the belief that the HOMO (LUMO) are localized on N (B). This is due to the larger electronegativity of C as compared to B. In the NCN system HOMO and LUMO



are localized mainly on the C-C bonds (with different orientation for HOMO and LUMO) and are partially localized on the adjacent N atoms and the B atoms never contribute.

The special shape of the localized HOMO and LUMO states around the two ends of the C-line for the NCB is of most interest. The HOMO orbitals in NCB are localized over a few top C-C bonds and neighbor B atoms while for the LUMO we notice that they are localized over a few bottom C-C bonds where B (N) atoms in the RHS (LHS partially) are mainly contributing with different shape as compared to the HOMO. It is important to emphasize that: i) we found the same orbital distribution in a BN system when it is doped by an arm-chair line of carbon atoms in the middle (those results are not reported in this paper), and ii) we did not find such orbitals employing semi-infinite NCB, i.e. a ribbon with periodic boundary along the C-line. The special shape of HOMO and LUMO orbitals found in NCB are not found in the BN system [9, 10].

Next we will focus on the NCB system to study its response to an external electric field. When an electric field in the opposite direction of the dipole moment of the NCB is applied, the gap becomes smaller, see Fig. 6(a), and the HOMO (LUMO) is localized much closer to the top (bottom), see Fig. 6(c). On the other hand, we found in the previous section that the electric polarizability in response to an external field is increased by doping the BNNRs by carbon atoms. This trend can be used to obtain metallic properties in doped NCB. Insertion of different numbers of carbon lines as well as using different arrangements of the atoms near the C-line can be a practical tool to tune the electric transmission through the BNNRs and their metallic properties.

An external uniform electric field  $E_y$  along the C-line in NCB causes a potential difference along the C-line. We assume that the HOMO and the LUMO are effectively centered around  $y_H$  and  $y_L$ , respectively. An applied electric field ( $E_y$ ) can modulate the energy gap as  $(y_L - y_H)eE_y$ , where  $e$  is the elementary charge. The gap can be tuned by the strength and direction of the electric field. The latter linear behavior is obtained even using the LDA (see top inset in Fig. 6(a)) and is continued (with a slope of  $(y_L - y_H)e$ ) while the centers of the HOMO and the LUMO are more or less fixed which is the case even for a rather strong field of  $E=+0.82$  V/nm (compare Fig. 3(b) and Fig. 6(c)). The

same linear behavior is found for the reverse electric fields  $E_y > -0.8$  V/nm, see Fig. 6(a).

On the other hand, if a strong negative field about  $-1$  V/nm is applied, the dependence is no longer linear. Fig. 6(b) shows that such a negative field alters the spatial distribution of the orbitals and elongates both HOMO and LUMO into a non-localized distribution similar to those found for the BCB or NCN systems. Therefore around the maximum,  $y_L \approx y_H$  and the energy gap is independent of the field strength. However for the negative fields beyond the maximum the energy gap decreases which corresponds to the localization of the LUMO and the HOMO where  $y_L < y_H$ . This simple picture argues that  $(y_L - y_H)eE_y$  modulates the energy-gap. Notice that the slope  $(y_L - y_H)e$  changes sign passing the maximum ( $E_y \simeq -1$  V/nm), therefore by decreasing the electric field, the gap decreases when  $E_y \succeq -1$  V/nm and increases when  $E_y \preceq -1.0$  V/nm. A similar behavior was found for a semi-infinite non-doped BN systems [9, 10], with difference in maximum and energy gap values. The bottom inset in Fig. 6(a) shows the variation of the HOMO and LUMO states with the electric field. We believe that the control of the conductivity by an external field as we found for the NCB will be of great practical interest.

In summary, we studied the electronic properties of boron-nitride sheets in the presence of a zigzag atomic line of carbon atoms in the middle of the BN sheets. Electronic polarization of the BNNRs was found to depend on the local arrangement of the boron and nitrogen atoms around the carbon line. Doping with carbon atoms decreases the non-metallic properties of the BNNRs by reducing the energy gap and increasing the polarizability. By applying an electric field along the carbon line we showed that the dipole moment of BNNR induced by the carbon dopants can be reduced and even eliminated. This also reduces the energy gap in the electron spectrum and allows one to control the conductivity with an external field.

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TABLE I: Bond lengths in Å, atomic charge in e, HOMO-LUMO band gap in eV and spontaneous electric dipole moment  $P_0$  in D for the four studied nanoribbons in Fig. 1. Results for the gap are given for both B3LYP and LDA (respectively calculated by G09 and BigDFT).

Nanoribbon	$d_{B-N}$	$d_{B-C}$	$d_{N-C}$	$d_{C-C}$	$e_B$	$e_N$	$e_{C-B}$	$e_{C-N}$	gap:B3LYP	LDA	$P_o$ :B3LYP
BN	1.45	-	-	-	1.17	-1.17	-	-	5.69	3.85	10.8
NCB	1.45	1.55	1.41	1.40	1.01	-0.89	-0.47	0.32	1.52	0.39	44.24
BCB	1.45	1.57	-	1.46	1.041	-1.16	-0.28	-	1.47	0.60	0.08
NCN	1.45	-	1.43	1.39	1.15	-0.09	-	0.13	1.47	0.46	0.27

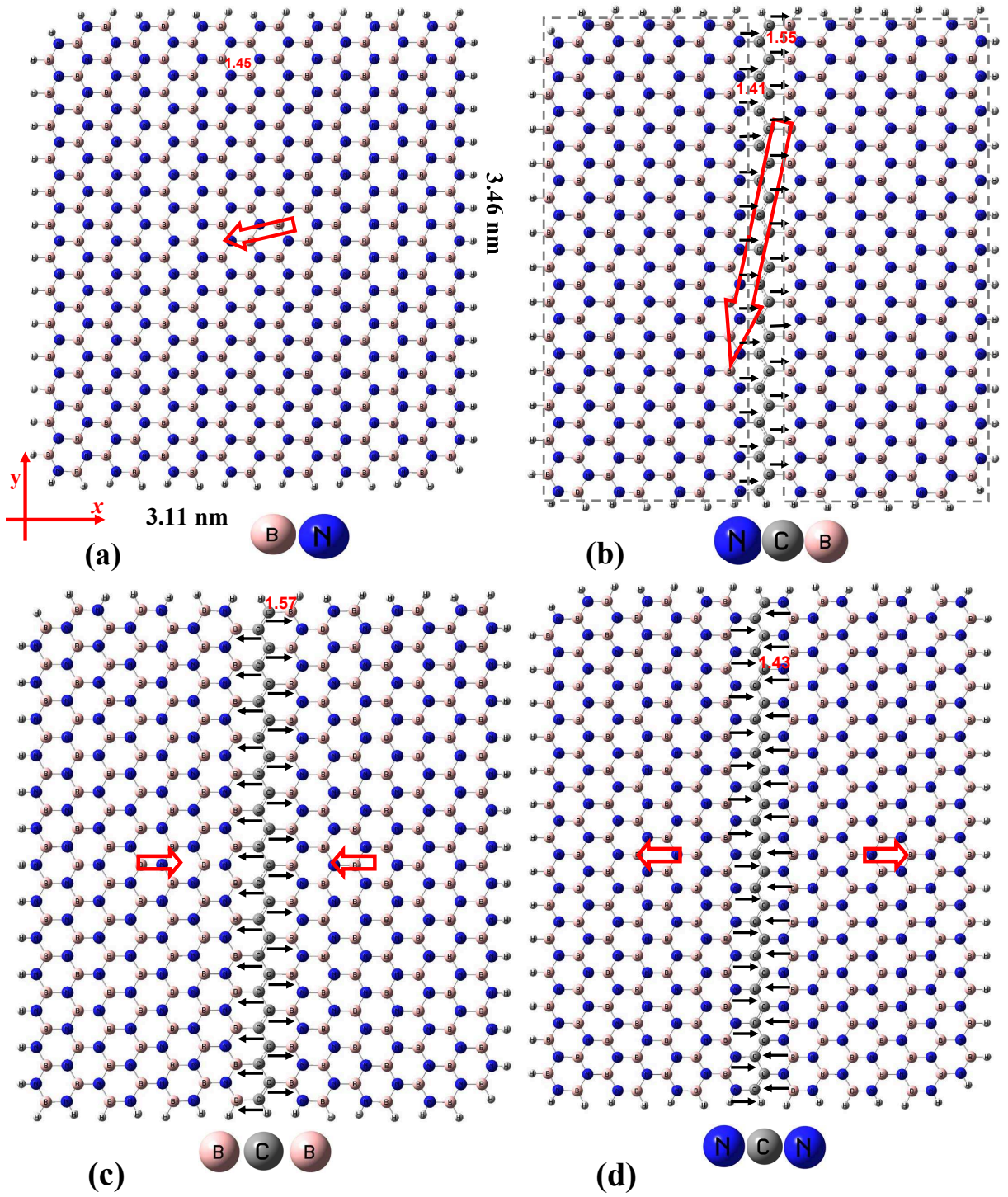
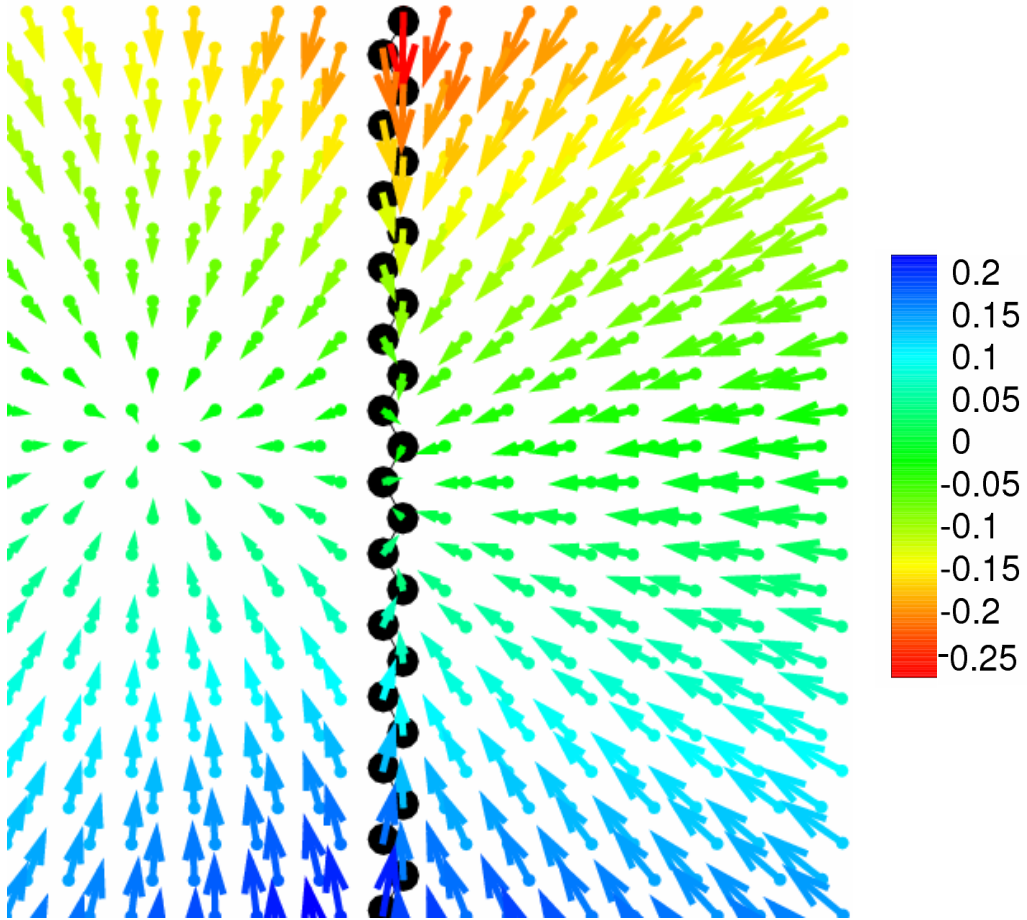


FIG. 1: (Color online) (a) Perfect boron-nitride nanoribbon (BN). (b) Boron-nitride nanoribbon with a zigzag C-line in the middle surrounded by both boron and nitrogen atoms on both sides (NCB). (c) Boron-nitride nanoribbons with the C-line surrounded only by boron atoms on both sides (BCB). (d) Boron-nitride nanoribbons with the C-line surrounded only by nitrogen atoms on both sides (NCN). In (a) and (b) red arrows refer to the total dipole moment of the systems and in (c), (d) red arrows refer to the total dipole moment on the two sides. The black horizontal arrows refer to the local dipoles corresponding to the B-C or N-C bonds. The simulated systems has size  $3.46 \times 3.11 \text{ nm}^2$  (Fig. 1). Numbers refer to the bond lengths in Å unit.



NCB

FIG. 2: (Color online) Atomic displacement after inserting an atomic carbon line in the middle of the BN sheet, i.e. NCB. The color coding indicates the y-component of the displacement vector, i.e. red (blue)  $\equiv$  downward (upward) displacement.



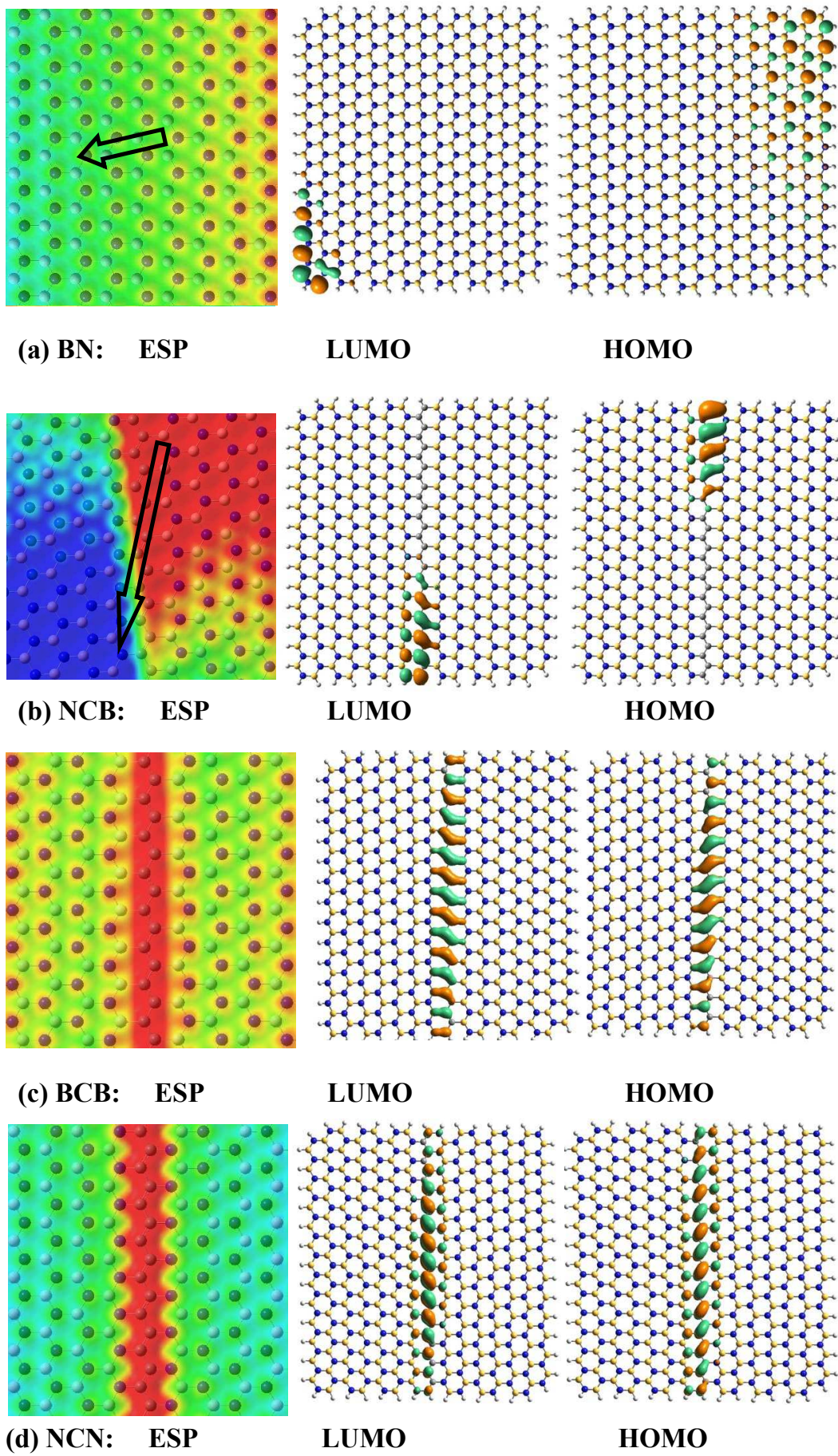


FIG. 3: (Color online) Contour plots of the electrostatic potential (ESP) for the four systems of Fig. 1 and the corresponding highest occupied molecular orbitals (HOMO) and the lowest unoccupied molecular orbital (LUMO). In (a) and (b) the black arrows refer to the total dipole moment.



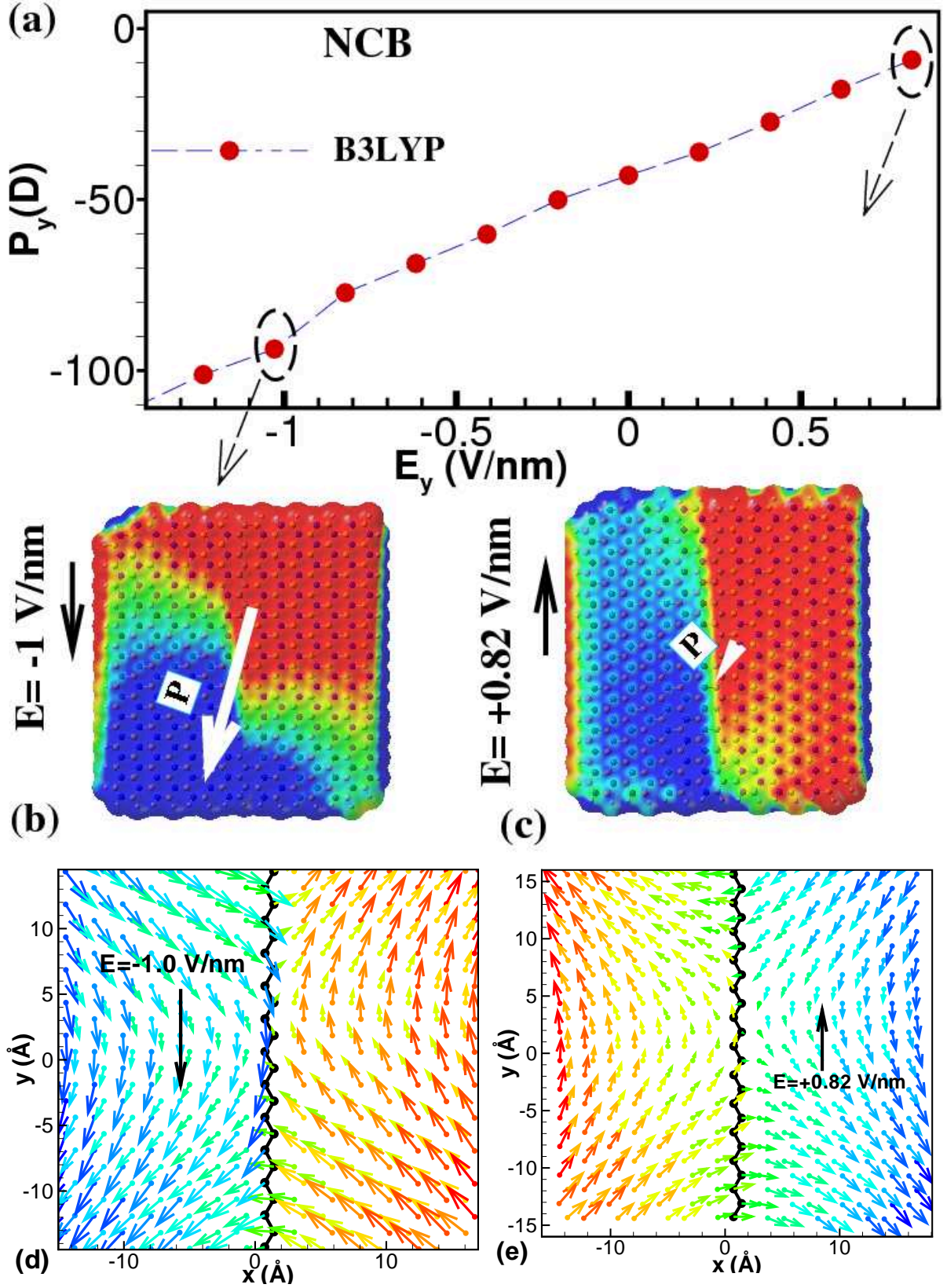


FIG. 4: (Color online) (a) Electric dipole moment versus applied electric field, both in the  $y$ -direction, for the NCB system using B3LYP functional. The corresponding ESPs and lattice deformation for  $E = E_y = -1.0$  V/nm (b,d) and  $E = E_y = +0.82$  V/nm (c,e). The black arrows (symbols) refer to the direction of the applied electric field (carbon atoms) and the white arrows refer to the total dipole moment.

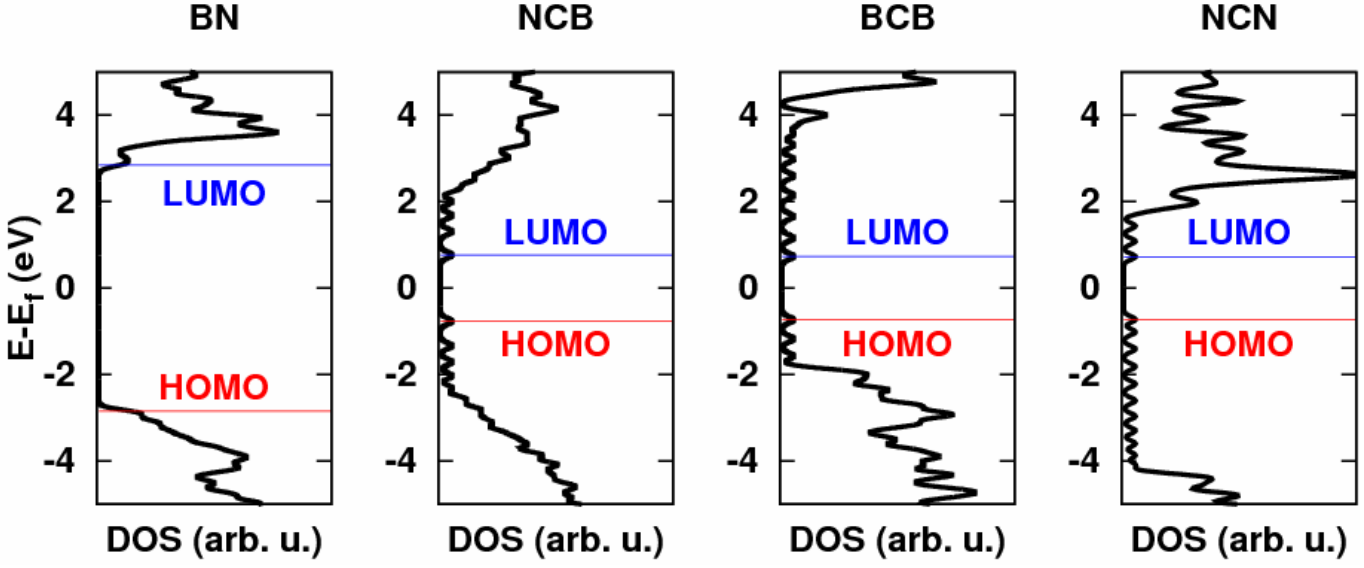


FIG. 5: (Color online) Density of states (DOS) for the four model systems. The presence of the carbon lines in the middle of the systems decreases the gap and modifies the DOS in different ways for each particular cases.

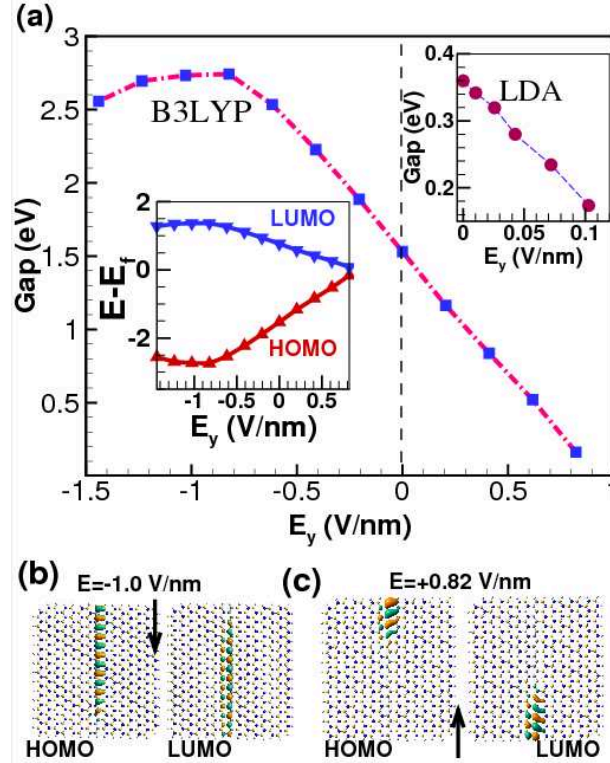


FIG. 6: (Color online) (a) The HOMO-LUMO energy gap for NCB versus applied electric field using B3LYP. Bottom inset shows the change in HOMO and LUMO versus applied electric field and the top inset shows the LDA results for positive electric field. The change in the HOMO and LUMO orbitals of NCB in the presence of electric field  $E_y = -1.0$  V/nm (b) (+0.82 V/nm (c)).